Author index

Alikhani, E.M., see Krim, L.	254 (2000) 267
Aloisio, S., and J.S. Francisco, A density functional study of H ₂ O-OClO,	
(H ₂ O) ₂ –OClO and H ₂ O–ClOO complexes	254 (2000) 1
Angulo, G., see Galán, M.	254 (2000) 329
Azria, R., see Tronc, M.	254 (2000) 69
Balta, B., and F.A. Gianturco, Structural properties and quantum effects in protonated	Market and a second
helium clusters. I. The ab initio interaction potential	254 (2000) 203
Balta, B., F.A. Gianturco and F. Paesani, Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller	
aggregates	254 (2000) 215
Baranović, G., see Stepanić, V.	254 (2000) 151
Basilevsky, M.V., see Vener, M.V.	254 (2000) 249
Baumgarten, M., see Karabunarliev, S.	254 (2000) 239
Bibinov, N.K., A.A. Fateev, D.B. Kokh, E.V. Lugovoj and A.M. Pravilov, Optical	
transitions from the chlorine $0_{11}^{+}(^{3}P_{2})$ ion-pair state	254 (2000) 89
Bliß, B., U. Lommatzsch, C. Monte, W. Rettig and B. Brutschy, Supersonic jet and	
solution studies of intramolecular complexes with TICT formation mimicking	
solute-solvent interaction	254 (2000) 407
Bonamy, J., see Bruet, X.	254 (2000) 297
Borras-Almenar, J.J., J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S. Tsukerblat, Anisotropic double exchange in orbitally degenerate mixed valence	
systems	254 (2000) 275
Boullant, E., see Chevreau, H.	254 (2000) 99
Bruet, X., J. Bonamy and M.L. Dubernet-Tuckey, Broadening and shifting coefficients	
of Raman isotropic $Q(j)(j=0,1,2)$ lines for pure H_2 : coupled states and semiclassical	
calculations. Comparison with experiments	254 (2000) 297
Brutschy, B., see Bliß, B.	254 (2000) 407
Cabaleiro-Lago, E.M., and M.A. Ríos, Ab initio study of M(CH ₃ CN) _n clusters	
(M=Li ⁺ , Na ⁺ , Mg ²⁺) in the gas phase	254 (2000) 11
Cabaleiro-Lago, E.M., see García-Muruais, A.	254 (2000) 109
Castaño, F., see Merelas, I.	254 (2000) 77
Cataliotti, R.S., see Morresi, A.	254 (2000) 337
Chen, M., see Zhang, L.	254 (2000) 231

Chevreau, H., E. Boullant, C. Dézarnaud-Dandine and A. Sevin, A theoretical	
exploratory study of low-energy (1-2 eV) electron catalysis in the $CO_2+H_2\rightarrow$	
HCOOH gas phase process	254 (2000) 99
Cisowski, J., see Mazurak, Z.	254 (2000) 25
Clemente-Juan, J.M., see Borras-Almenar, J.J.	254 (2000) 275
Cloutier, P., see Tronc, M.	254 (2000) 69
Coronado, E., see Borras-Almenar, J.J.	254 (2000) 275
Czaja, M., see Mazurak, Z.	254 (2000) 25
Dézarnaud-Dandine, C., see Chevreau, H.	254 (2000) 99
Derecskei-Kovacs, A., see Li, R.	254 (2000) 309
Dimitrova, Y., and S. Peyerimhoff, Ab initio study of structures of hydrogen-bonded	
nitric acid complexes	254 (2000) 125
Dubernet-Tuckey, M.L., see Bruet, X.	254 (2000) 297
Edvardsson, D., see Potts, A.W.	254 (2000) 385
Fateev, A.A., see Bibinov, N.K.	254 (2000) 89
Faure, A., L. Wiesenfeld and P. Valiron, Temperature dependence of fast neutral-	251 (2000) 05
neutral reactions: a triatomic model study	254 (2000) 49
Fedorov, A.V., and D.L. Snavely, Direct correlation method for OH, NH and CH local	20. (2000)
modes: vibrational overtone spectroscopy of biphenyl, anthracene, isobutanol,	
2-chloroethanol and ethylenediamine at the third overtone region	254 (2000) 169
Feller, KH., see Malyshev, V.A.	254 (2000) 31
Fernández, J.A., see Merelas, I.	254 (2000) 77
Francisco, J.S., see Aloisio, S.	254 (2000) 1
Galán, M., and G. Angulo, Some remarks on the application of relaxation techniques	
to chemical equilibria	254 (2000) 329
Galasso, V., D. Jones, A. Modelli and M.L. Trudell, A study of the molecular structure	
and spectroscopic properties of benzo- and pyrido-tetraazapentalenes	254 (2000) 375
García-Muruais, A., E.M. Cabaleiro-Lago, J.M. Hermida-Ramón and M.A. Ríos, The study of A(CH ₃ OH) ₁₋₆ (A=Li ⁺ , Na ⁺) in the gas phase based on ab initio	
calculations, analysis of the solvation process	254 (2000) 109
Ghosh, S.K., see Samanta, A.	254 (2000) 39
Gianturco, F.A., see Balta, B.	254 (2000) 203
Gianturco, F.A., see Balta, B.	254 (2000) 215
Glaeske, H., see Malyshev, V.A.	254 (2000) 31
Glasbeek, M., see Humbs, W.	254 (2000) 319
Gratz, H., and A. Penzkofer, Singlet-singlet excited-state absorption and triplet-triplet	20 (2000) 512
absorption of meso-tetraphenylporphine	254 (2000) 363
Hayes, M.A., see Potts, A.W.	254 (2000) 385
Heimann, J., see Mazurak, Z.	254 (2000) 25
Hermida-Ramón, J.M., see García-Muruais, A.	254 (2000) 109
Holland, D.M.P., see Potts, A.W.	254 (2000) 385
Humbs, W., H. Zhang and M. Glasbeek, Femtosecond fluorescence upconversion	
spectroscopy of vapor-deposited tris(8-hydroxyquinoline) aluminum films	254 (2000) 319
Husain, D., see Merelas, I.	254 (2000) 77

Jones, D., see Galasso, V.	254 (2000) 375
Küpper, J., see Schmitt, M.	254 (2000) 349
Karabunarliev, S., and M. Baumgarten, Using antiferromagnetic couplers for high-spir	, ,
ground states in ion radicals	254 (2000) 239
Karlsson, L., see Potts, A.W.	254 (2000) 385
	, , ,
Kokh, D.B., see Bibinov, N.K.	254 (2000) 89
Kozlov, G.G., see Malyshev, V.A.	254 (2000) 31
Krim, L., C. Prot, E.M. Alikhani and L. Manceron, Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR matrix isolation study	254 (2000) 267
Le Coat, Y., see Tronc, M.	254 (2000) 69
Li, R., A. Derecskei-Kovacs and S.W. North, The unimolecular dissociation of 2- butenenitrile: measurements of the CN elimination channel using FM Doppler	alliantia tattiini
spectroscopy	254 (2000) 309
Lommatzsch, U., see Bliß, B.	254 (2000) 407
Lugovoj, E.V., see Bibinov, N.K.	254 (2000) 89
MacDonald, M.A., see Potts, A.W.	254 (2000) 385
Malyshev, V.A., G.G. Kozlov, H. Glaeske and KH. Feller, Channels of the exciton-	, ,
exciton annihilation in one-dimensional aggregates at low temperature	254 (2000) 31
Manceron, L., see Krim, L.	254 (2000) 267
Maripuu, R., see Potts, A.W.	254 (2000) 385
Mazurak, Z., J. Cisowski, J. Heimann, A. Nateprov and M. Czaja, Magnetic	
susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium Merelas, I., J.A. Fernández, P. Puyuelo, M.N. Sánchez Rayo, D. Husain and F. Castaño, The collisional removal of the carbene CCl ₂ (X(0,0,0)) and	254 (2000) 25
$CCl_2(\tilde{A}^1B_1(0,7,0))$ by rare gases and simple molecules	254 (2000) 77
Modelli, A., see Galasso, V.	254 (2000) 375
Monte, C., see Bliß, B.	254 (2000) 407
Morresi, A., P. Sassi, M. Paolantoni, S. Santini and R.S. Cataliotti, Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes in liquid	
acetonitrile and acetonitrile-d ₃	254 (2000) 337
Nateprov, A., see Mazurak, Z.	254 (2000) 25
North, S.W., see Li, R.	254 (2000) 309
Paesani, F., see Balta, B.	254 (2000) 215
Palii, A.V., see Borras-Almenar, J.J.	254 (2000) 275
Paolantoni, M., see Morresi, A.	254 (2000) 275 254 (2000) 337
Penzkofer, A., see Gratz, H.	*
	254 (2000) 363
Petsalakis, I.D., and G. Theodorakopoulos, Electronic states of CF ⁺	254 (2000) 181
Peyerimhoff, S., see Dimitrova, Y.	254 (2000) 125
Potts, A.W., D. Edvardsson, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von Niessen, An experimental and	
theoretical study of the valence shell photoelectron spectrum of the chlorobenzene	
theoretical study of the valence shell photoelectron spectrum of the chlorobenzene molecule	254 (2000) 385

Prot, C., see Krim, L.	254 (2000) 267
Puyuelo, P., see Merelas, I.	254 (2000) 77
Qin, QZ., see Zhang, L.	254 (2000) 231
Ríos, M.A., see Cabaleiro-Lago, E.M.	254 (2000) 11
Ríos, M.A., see García-Muruais, A.	254 (2000) 109
Rettig, W., see Bliß, B.	254 (2000) 407
Rostov, I.V., see Vener, M.V.	254 (2000) 249
Sánchez Rayo, M.N., see Merelas, I.	254 (2000) 77
Samanta, A., and S.K. Ghosh, Role of inertial and non-Markovian effects on activated	The Column of th
barrier crossing dynamics for charge transfer reactions in solution	254 (2000) 39
Sanche, L., see Tronc, M.	254 (2000) 69
Santini, S., see Morresi, A.	254 (2000) 337
Sassi, P., see Morresi, A.	254 (2000) 337
Schmitt, M., J. Küpper, D. Spangenberg and A. Westphal, Determination of the	
structures and barriers to hindered internal rotation of the phenol-methanol cluster	251 (2000) 210
in the S_0 and S_1 states	254 (2000) 349
Sevin, A., see Chevreau, H.	254 (2000) 99
Siegbahn, K., see Potts, A.W.	254 (2000) 385
Snavely, D.L., see Fedorov, A.V.	254 (2000) 169
Soudackov, A.V., see Vener, M.V.	254 (2000) 249
Spangenberg, D., see Schmitt, M.	254 (2000) 349
Spanget-Larsen, J., E.W. Thulstrup and J. Waluk, Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular dichroism, and quantum chemical	
calculations	254 (2000) 135
Stepanić, V., and G. Baranović, Ground and excited states of isodiazene - an ab initio	
study	254 (2000) 151
Theodorakopoulos, G., see Petsalakis, I.D.	254 (2000) 181
Thulstrup, E.W., see Spanget-Larsen, J.	254 (2000) 135
Tronc, M., R. Azria, Y. Le Coat, P. Cloutier and L. Sanche, Kinetic energy distributions for O ⁻ and metastable CO [*] produced by electron stimulated desorption	254 (2000) 155
from condensed CO ₂	254 (2000) 69
Trudell, M.L., see Galasso, V.	254 (2000) 375
Tsukerblat, B.S., see Borras-Almenar, J.J.	
Isukerbiat, B.S., see Borras-Ameriar, J.J.	254 (2000) 275
Valiron, P., see Faure, A.	254 (2000) 49
Vener, M.V., I.V. Rostov, A.V. Soudackov and M.V. Basilevsky, Semiempirical	
modeling free energy surfaces for proton transfer in polar aprotic solvents	254 (2000) 249
von Niessen, W., see Potts, A.W.	254 (2000) 385
Waluk, J., see Spanget-Larsen, J.	254 (2000) 135
Wang, X., see Zhang, L.	254 (2000) 231
Westphal, A., see Schmitt, M.	
Wiesenfeld, L., see Faure, A.	254 (2000) 49
	254 (2000) 49
You, XZ., see Zhu, XL.	254 (2000) 287

Zanchini, C., Silylcyanides and silylisocyanides: a comparative theoretical study	254 (2000) 187
Zhang, H., see Humbs, W.	254 (2000) 319
Zhang, L., X. Wang, M. Chen and QZ. Qin, Activation of CO2 by Zr atom. Matrix-	
isolation FTIR spectroscopy and density functional studies	254 (2000) 231
Zhang, Y., see Zhu, XL.	254 (2000) 287
Zhu, XL., XZ. You and Y. Zhang, A novel approach to calculation of the second-order nonlinear optical susceptibilities of organic crystals based on energy-band	
theory	254 (2000) 287



Subject index

Methods and constructs

Theoretical

Computational methods for electronic structure	
A density functional study of H ₂ O-OClO, (H ₂ O) ₂ -OClO and H ₂ O-ClOO complexes, S.	
Aloisio and J.S. Francisco	254 (2000) 1
Ab initio study of $M(CH_3CN)_n$ clusters $(M=Li^+, Na^+, Mg^{2+})$ in the gas phase, E.M.	
Cabaleiro-Lago and M.A. Ríos	254 (2000) 11
Magnetic susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium,	
Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja	254 (2000) 25
A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the	
CO ₂ +H ₂ →HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud-	
Dandine and A. Sevin	254 (2000) 99
The study of A(CH ₃ OH) ₁₋₆ (A=Li ⁺ , Na ⁺) in the gas phase based on ab initio	
calculations, analysis of the solvation process, A. García-Muruais, E.M. Cabaleiro-	
Lago, J.M. Hermida-Ramón and M.A. Ríos	254 (2000) 109
Ab initio study of structures of hydrogen-bonded nitric acid complexes, Y. Dimitrova	
and S. Peyerimhoff	254 (2000) 125
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular	
dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup	
and J. Waluk	254 (2000) 135
Ground and excited states of isodiazene - an ab initio study, V. Stepanić and G.	
Baranović	254 (2000) 151
Direct correlation method for OH, NH and CH local modes: vibrational overtone spectroscopy of biphenyl, anthracene, isobutanol, 2-chloroethanol and ethylenedia-	
mine at the third overtone region, A.V. Fedorov and D.L. Snavely	254 (2000) 169
Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini	254 (2000) 187
Structural properties and quantum effects in protonated helium clusters. I. The ab initio	
interaction potential, B. Balta and F.A. Gianturco	254 (2000) 203
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S.	
Karabunarliev and M. Baumgarten	254 (2000) 239
	(

-CI and valence bond approach Electronic states of CF ⁺ , I.D. Petsalakis and G. Theodorakopoulos	254 (2000) 181
-density functional theory	
Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini Structural properties and quantum effects in protonated helium clusters. I. The ab initio	254 (2000) 187
interaction potential, B. Balta and F.A. Gianturco Activation of CO ₂ by Zr atom. Matrix-isolation FTIR spectroscopy and density	254 (2000) 203
functional studies, L. Zhang, X. Wang, M. Chen and QZ. Qin	254 (2000) 231
Semiempirical methods	
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S. Karabunarliev and M. Baumgarten	254 (2000) 239
Semiempirical modeling free energy surfaces for proton transfer in polar aprotic solvents, M.V. Vener, I.V. Rostov, A.V. Soudackov and M.V. Basilevsky	254 (2000) 249
Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron	254 (2000) 267
Spin states and magnetic interactions Magnetic susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium,	
Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja Anisotropic double exchange in orbitally degenerate mixed valence systems, J.J. Borras-	254 (2000) 25
Almenar, J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S. Tsukerblat	254 (2000) 275
Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)	
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller	254 (2000) 31
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup	
and J. Waluk	254 (2000) 135
A novel approach to calculation of the second-order nonlinear optical susceptibilities of organic crystals based on energy-band theory, XL. Zhu, XZ. You and Y. Zhang	254 (2000) 287
Radiative (incl. relativistic) effects on molecules and molecular processes	
Broadening and shifting coefficients of Raman isotropic $Q(j)(j=0,1,2)$ lines for pure H_2 : coupled states and semiclassical calculations. Comparison with experiments, X .	
Bruet, J. Bonamy and M.L. Dubernet-Tuckey	254 (2000) 297
Scattering of waves and particles	
Broadening and shifting coefficients of Raman isotropic $Q(j)(j=0,1,2)$ lines for pure H_2 : coupled states and semiclassical calculations. Comparison with experiments, X .	254 (2000) 207
Bruet, J. Bonamy and M.L. Dubernet-Tuckey	254 (2000) 297
Intramolecular dynamics	
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W.	
North	254 (2000) 309

Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek	254 (2000) 319
Molecular dynamics of many particle systems and condensed phases	
Molecular dynamics of many particle systems and condensed phases Role of inertial and non-Markovian effects on activated barrier crossing dynamics for charge transfer reactions in solution, A. Samanta and S.K. Ghosh	254 (2000) 39
Statistical computational methods (incl. Monte Carlo)	
Temperature dependence of fast neutral-neutral reactions: a triatomic model study, A. Faure, L. Wiesenfeld and P. Valiron	254 (2000) 49
Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F.	Zi pigamaligasi
Paesani	254 (2000) 215
Dynamics of structures, lattices and macromolecular conformations	
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller	254 (2000) 31
Fluctuations and random processes	
Some remarks on the application of relaxation techniques to chemical equilibria, M. Galán and G. Angulo	254 (2000) 329
Non-equilibrium statistical mechanics Role of inertial and non-Markovian effects on activated barrier crossing dynamics for charge transfer reactions in solution, A. Samanta and S.K. Ghosh	254 (2000) 39
Experiment	
Magnetic resonances	
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S. Karabunarliev and M. Baumgarten	254 (2000) 239
Molecular spectroscopy	
The collisional removal of the carbene $CCl_2(\tilde{X}(0,0,0))$ and $CCl_2(\tilde{A}^1B_1(0,7,0))$ by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez	
Rayo, D. Husain and F. Castaño	254 (2000) 77
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup	
and J. Waluk	254 (2000) 135
Ground and excited states of isodiazene – an ab initio study, V. Stepanić and G. Baranović	254 (2000) 151
Some remarks on the application of relaxation techniques to chemical equilibria, M.	254 (2000) 151
Galán and G. Angulo	254 (2000) 329
Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes in liquid acetonitrile and acetonitrile-d ₃ , A. Morresi, P. Sassi, M. Paolantoni, S.	
Santini and R.S. Cataliotti	254 (2000) 337

Determination of the structures and barriers to hindered internal rotation of the	
phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal	254 (2000) 349
-infrared	
Activation of CO ₂ by Zr atom. Matrix-isolation FTIR spectroscopy and density functional studies, L. Zhang, X. Wang, M. Chen and QZ. Qin Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR	254 (2000) 231
matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron	254 (2000) 267
-visible	
Singlet-singlet excited-state absorption and triplet-triplet absorption of meso-tetra- phenylporphine, H. Gratz and A. Penzkofer	254 (2000) 363
Photoelectron and Auger spectroscopy	
A study of the molecular structure and spectroscopic properties of benzo- and pyrido- tetraazapentalenes, V. Galasso, D. Jones, A. Modelli and M.L. Trudell	254 (2000) 375
An experimental and theoretical study of the valence shell photoelectron spectrum of the chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von	and and the second
Niessen	254 (2000) 385
Multiphoton ionization Supersonic jet and solution studies of intramolecular complexes with TICT formation mimicking solute—solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig and B. Brutschy	254 (2000) 407
Electron impact spectroscopy	
Kinetic energy distributions for O ⁻ and metastable CO [*] produced by electron stimulated desorption from condensed CO ₂ , M. Tronc, R. Azria, Y.L. Coat, P.	
Cloutier and L. Sanche	254 (2000) 69
Laser induced fluorescence	
The collisional removal of the carbene $CCl_2(\tilde{X}(0,0,0))$ and $CCl_2(\tilde{A}^1B_1(0,7,0))$ by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez	
Rayo, D. Husain and F. Castaño	254 (2000) 77
Optical transitions from the chlorine 0 _u ⁺ (³ P ₂) ion-pair state, N.K. Bibinov, A.A. Fateev, D.B. Kokh, E.V. Lugovoj and A.M. Pravilov	254 (2000) 89
Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal	254 (2000) 349
Supersonic jet and solution studies of intramolecular complexes with TICT formation	254 (2000) 549
mimicking solute-solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig and B. Brutschy	254 (2000) 407
Ultrafast measurements	
Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-	
hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek	254 (2000) 319

Subject maex r Chemical Physics 254 (2000) 427-456	431
Singlet-singlet excited-state absorption and triplet-triplet absorption of meso-tetra-	
phenylporphine, H. Gratz and A. Penzkofer	254 (2000) 363
Nonlinear optics and spectroscopy	
Singlet-singlet excited-state absorption and triplet-triplet absorption of meso-tetra-	
phenylporphine, H. Gratz and A. Penzkofer	254 (2000) 363
Synchrotron spectroscopies	
An experimental and theoretical study of the valence shell photoelectron spectrum of the chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von	
Niessen	254 (2000) 385
Optical pumping	
Magnetic susceptibility and luminescence of α -ZnAl ₂ S ₄ tiospinel doped with chromium,	
Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja	254 (2000) 25
Optoacoustic spectroscopy	
Direct correlation method for OH, NH and CH local modes: vibrational overtone	
spectroscopy of biphenyl, anthracene, isobutanol, 2-chloroethanol and ethylenedia-	
mine at the third overtone region, A.V. Fedorov and D.L. Snavely	254 (2000) 169
Mass spectroscopy	
Kinetic energy distributions for O and metastable CO produced by electron	
stimulated desorption from condensed CO2, M. Tronc, R. Azria, Y. Le Coat, P.	
Cloutier and L. Sanche	254 (2000) 69
Measurement of macroscopic variables	
Some remarks on the application of relaxation techniques to chemical equilibria, M.	
Galán and G. Angulo	254 (2000) 329
Objects	
Bulk systems	
Gases	
The collisional removal of the carbene $CCl_2(\tilde{X}(0,0,0))$ and $CCl_2(\tilde{A}^1B_1(0,7,0))$ by rare	
gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez	
Rayo, D. Husain and F. Castaño	254 (2000) 77
Optical transitions from the chlorine $0_u^+(^3P_2)$ ion-pair state, N.K. Bibinov, A.A. Fateev,	254 (2000) 80
D.B. Kokh, E.V. Lugovoj and A.M. Pravilov	254 (2000) 89
Ground and excited states of isodiazene – an ab initio study, V. Stepanić and G. Baranović	254 (2000) 151
Structural properties and quantum effects in protonated helium clusters. I. The ab initio	254 (2000) 151
interaction potential, B. Balta and F.A. Gianturco	254 (2000) 203

Structural properties and quantum effects in protonated helium clusters. II. Quantum	
Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F.	
Paesani	254 (2000) 215
Broadening and shifting coefficients of Raman isotropic $Q(j)(j=0,1,2)$ lines for pure	
H ₂ : coupled states and semiclassical calculations. Comparison with experiments, X.	
Bruet, J. Bonamy and M.L. Dubernet-Tuckey	254 (2000) 297
Transmittation of School & Wint 18 (September 1988)	()
Supersonic beams	
Supersonic jet and solution studies of intramolecular complexes with TICT formation	
mimicking solute-solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig	
and B. Brutschy	254 (2000) 407
and D. Didistriy	201 (2000) 107
Liquid mixtures and solutions	
Role of inertial and non-Markovian effects on activated barrier crossing dynamics for	
charge transfer reactions in solution, A. Samanta and S.K. Ghosh	254 (2000) 39
Semiempirical modeling free energy surfaces for proton transfer in polar aprotic	254 (2000) 57
solvents, M.V. Vener, I.V. Rostov, A.V. Soudackov and M.V. Basilevsky	254 (2000) 249
	234 (2000) 249
Some remarks on the application of relaxation techniques to chemical equilibria, M.	254 (2000) 220
Galán and G. Angulo	254 (2000) 329
Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes	
in liquid acetonitrile and acetonitrile-d ₃ , A. Morresi, P. Sassi, M. Paolantoni, S.	
Santini and R.S. Cataliotti	254 (2000) 337
Crystals	
Magnetic susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium,	
Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja	254 (2000) 25
A novel approach to calculation of the second-order nonlinear optical susceptibilities of	254 (2000) 25
	254 (2000) 297
organic crystals based on energy-band theory, XL. Zhu, XZ. You and Y. Zhang	254 (2000) 287
Complex fluids	
Role of inertial and non-Markovian effects on activated barrier crossing dynamics for	
charge transfer reactions in solution, A. Samanta and S.K. Ghosh	254 (2000) 39
	20. (2000)
Polymers	
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular	
dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup	
and J. Waluk	254 (2000) 135
	251 (2000) 155
Thin films	
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low	
temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller	254 (2000) 31
Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-	(
hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek	254 (2000) 319
	(2000) 000
Surfaces	
Kinetic energy distributions for O and metastable CO produced by electron	
stimulated desorption from condensed CO ₂ , M. Tronc, R. Azria, Y. Le Coat, P.	
Cloutier and L. Sanche	254 (2000) 69
	20 (2000) 0)

Microscopic and mesoscopic systems

Molecules (neutral and ionic)		
Magnetic susceptibility and luminescence of α-ZnAl ₂ S ₄ tiospinel doped with chromium,		
Z. Mazurak, J. Cisowski, J. Heimann, A. Nateprov and M. Czaja	254 (2000) 2	25
Optical transitions from the chlorine $0^+_{11}(^3P_2)$ ion-pair state, N.K. Bibinov, A.A. Fateev,	251 (2000)	
D.B. Kokh, E.V. Lugovoj and A.M. Pravilov	254 (2000) 8	29
Direct correlation method for OH, NH and CH local modes: vibrational overtone	25 (2000)	,,
spectroscopy of biphenyl, anthracene, isobutanol, 2-chloroethanol and ethylenedia-		
mine at the third overtone region, A.V. Fedorov and D.L. Snavely	254 (2000) 16	59
Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini	254 (2000) 18	
Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes	254 (2000) 10	,,
in liquid acetonitrile and acetonitrile-d ₃ , A. Morresi, P. Sassi, M. Paolantoni, S.		
Santini and R.S. Cataliotti	254 (2000) 33	37
Summ and R.S. Catanotti	254 (2000) 55	,
diatomic		
Electronic states of CF ⁺ , I.D. Petsalakis and G. Theodorakopoulos	254 (2000) 18	31
Broadening and shifting coefficients of Raman isotropic $Q(j)$ ($j = 0,1,2$) lines for pure	20 (2000) 10	•
H_2 : coupled states and semiclassical calculations. Comparison with experiments, X.		
Bruet, J. Bonamy and M.L. Dubernet-Tuckey	254 (2000) 29	7
	20 . (2000) 22	
small polyatomics		
A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the		
CO ₂ +H ₂ →HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud-		
Dandine and A. Sevin	254 (2000) 9	9
Ground and excited states of isodiazene - an ab initio study, V. Stepanić and G.		
Baranović	254 (2000) 15	1
Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini	254 (2000) 18	
Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR		
matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron	254 (2000) 26	7
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination		
channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W.		
North	254 (2000) 30	9
	201 (2000) 20	
aromatics		
Electronic states of diphenyl- and dipyridyl-s-tetrazines: linear and magnetic circular		
dichroism, and quantum chemical calculations, J. Spanget-Larsen, E.W. Thulstrup and J. Waluk	254 (2000) 13:	5
inglet-singlet excited-state absorption and triplet-triplet absorption of meso-tetra-	254 (2000) 15.	9
	254 (2000) 363	2
phenylporphine, H. Gratz and A. Penzkofer	234 (2000) 30.	3
study of the molecular structure and spectroscopic properties of benzo- and pyrido-	254 (2000) 27	5
tetraazapentalenes, V. Galasso, D. Jones, A. Modelli and M.L. Trudell	254 (2000) 375)
an experimental and theoretical study of the valence shell photoelectron spectrum of		
the chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P.		
Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von	254 (2000) 204	5
Niessen	254 (2000) 385)

Molecular aggregates	
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller Temperature dependence of fast neutral-neutral reactions: a triatomic model study, A.	254 (2000) 31
Faure, L. Wiesenfeld and P. Valiron	254 (2000) 49
The study of A(CH ₃ OH) ₁₋₆ (A=Li ⁺ , Na ⁺) in the gas phase based on ab initio calculations, analysis of the solvation process, A. García-Muruais, E.M. Cabaleiro-Lago, J.M. Hermida-Ramón and M.A. Ríos	254 (2000) 109
Ab initio study of structures of hydrogen-bonded nitric acid complexes, Y. Dimitrova and S. Peyerimhoff	254 (2000) 125
Supersonic jet and solution studies of intramolecular complexes with TICT formation mimicking solute-solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig and B. Brutschy	254 (2000) 407
the quality week and not be a first of the second of the s	31 June internet
-dimers Anisotropic double exchange in orbitally degenerate mixed valence systems, J.J. Borras-	
Almenar, J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S. Tsukerblat	254 (2000) 275
-clusters	
Structural properties and quantum effects in protonated helium clusters. I. The ab initio interaction potential, B. Balta and F.A. Gianturco	254 (2000) 203
Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F.	254 (2000) 215
Paesani Determination of the structures and barriers to hindered internal rotation of the	254 (2000) 215
phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal	254 (2000) 349
-complexes A density functional study of H ₂ O-OClO, (H ₂ O) ₂ -OClO and H ₂ O-ClOO complexes, S.	
Aloisio and J.S. Francisco	254 (2000) 1
Ab initio study of M(CH ₃ CN) _n clusters (M=Li ⁺ , Na ⁺ , Mg ²⁺) in the gas phase, E.M.	
Cabaleiro-Lago and M.A. Ríos	254 (2000) 11
Semiempirical modeling free energy surfaces for proton transfer in polar aprotic solvents, M.V. Vener, I.V. Rostov, A.V. Soudackov and M.V. Basilevsky	254 (2000) 249
Free radicals (incl. hydronium and muonium)	
The collisional removal of the carbene $CCl_2(\tilde{X}(0,0,0))$ and $CCl_2(\tilde{A}^1B_1(0,7,0))$ by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez	
Rayo, D. Husain and F. Castaño	254 (2000) 77
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W.	254 (2000) 200
North	254 (2000) 309
Ions and charge carriers	
A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the	
CO ₂ +H ₂ →HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud- Dandine and A. Sevin	254 (2000) 99

Proteins

Some remarks on the application of relaxation techniques to chemical equilibria, M. Galán and G. Angulo

254 (2000) 329

Phenomena

Molecular structure A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the CO₂+H₂→HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud-Dandine and A. Sevin

254 (2000) 99

Ab initio study of structures of hydrogen-bonded nitric acid complexes, Y. Dimitrova and S. Peyerimhoff

254 (2000) 125

Silylcyanides and silylisocyanides: a comparative theoretical study, C. Zanchini

254 (2000) 187

Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani

254 (2000) 215

Activation of CO₂ by Zr atom. Matrix-isolation FTIR spectroscopy and density functional studies, L. Zhang, X. Wang, M. Chen and Q.-Z. Qin

254 (2000) 231

Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron

254 (2000) 267

Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal

254 (2000) 349

A study of the molecular structure and spectroscopic properties of benzo- and pyridotetraazapentalenes, V. Galasso, D. Jones, A. Modelli and M.L. Trudell

254 (2000) 375

Vibrations and rotations of molecules

A density functional study of H₂O-OClO, (H₂O)₂-OClO and H₂O-ClOO complexes, S. Aloisio and J.S. Francisco

254 (2000) 1

Direct correlation method for OH, NH and CH local modes: vibrational overtone spectroscopy of biphenyl, anthracene, isobutanol, 2-chloroethanol and ethylenediamine at the third overtone region, A.V. Fedorov and D.L. Snavely

254 (2000) 169

Activation of CO₂ by Zr atom. Matrix-isolation FTIR spectroscopy and density functional studies, L. Zhang, X. Wang, M. Chen and Q.-Z. Qin

254 (2000) 231

Broadening and shifting coefficients of Raman isotropic Q(j)(j=0,1,2) lines for pure H_2 : coupled states and semiclassical calculations. Comparison with experiments, X. Bruet, J. Bonamy and M.L. Dubernet-Tuckey

254 (2000) 297

Solvent effect on the vibrational dephasing of the v_2 (CN) and v_4 (CC) stretching modes in liquid acetonitrile and acetonitrile-d₃, A. Morresi, P. Sassi, M. Paolantoni, S. Santini and R.S. Cataliotti

254 (2000) 337

Electronic structure and states

The collisional removal of the carbene $CCl_2(\tilde{X}(0,0,0))$ and $CCl_2(\tilde{A}^1B_1(0,7,0))$ by rare gases and simple molecules, I. Merelas, J.A. Fernández, P. Puyuelo, M.N. Sánchez Rayo, D. Husain and F. Castaño

254 (2000) 77

Ground and excited states of isodiazene – an ab initio study, V. Stepanić and G.	
Baranović	254 (2000) 151
Electronic states of CF ⁺ , I.D. Petsalakis and G. Theodorakopoulos Structural properties and quantum effects in protonated helium clusters. I. The ab initio	254 (2000) 181
interaction potential, B. Balta and F.A. Gianturco Activation of CO ₂ by Zr atom. Matrix-isolation FTIR spectroscopy and density	254 (2000) 203
functional studies, L. Zhang, X. Wang, M. Chen and QZ. Qin	254 (2000) 231
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S.	
Karabunarliev and M. Baumgarten Anisotropic double exchange in orbitally degenerate mixed valence systems, J.J. Borras-	254 (2000) 239
Almenar, J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S. Tsukerblat A study of the molecular structure and spectroscopic properties of benzo- and pyrido-	254 (2000) 275
tetraazapentalenes, V. Galasso, D. Jones, A. Modelli and M.L. Trudell An experimental and theoretical study of the valence shell photoelectron spectrum of the chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P.	254 (2000) 375
Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von Niessen	254 (2000) 385
Spin splittings	
Using antiferromagnetic couplers for high-spin ground states in ion radicals, S.	
Karabunarliev and M. Baumgarten	254 (2000) 239
Molecular interactions	
Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the S_0 and S_1 states, M. Schmitt, J. Küpper, D. Spangenberg and A. Westphal	254 (2000) 349
Energy transfer processes	
Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris(8-hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek	254 (2000) 319
Molecular photophysical processes	
Singlet-singlet excited-state absorption and triplet-triplet absorption of meso-tetra- phenylporphine, H. Gratz and A. Penzkofer	254 (2000) 363
An experimental and theoretical study of the valence shell photoelectron spectrum of the chlorobenzene molecule, A.W. Potts, D. Edvardsson, L. Karlsson, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, R. Maripuu, K. Siegbahn and W. von	
Niessen	254 (2000) 385
Supersonic jet and solution studies of intramolecular complexes with TICT formation mimicking solute-solvent interaction, B. Bliß, U. Lommatzsch, C. Monte, W. Rettig	
and B. Brutschy	254 (2000) 407
Photochemistry	
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W.	
North	254 (2000) 309

Intramolecular dynamics

-radiationless transitions	
Optical transitions from the chlorine 0 _u ⁺ (³ P ₂) ion-pair state, N.K. Bibinov, A.A. Fateev, D.B. Kokh, E.V. Lugovoj and A.M. Pravilov	254 (2000) 89
Luminescence spectra, yields and lifetimes	
Femtosecond fluorescence upconversion spectroscopy of vapor-deposited tris (8-hydroxyquinoline) aluminum films, W. Humbs, H. Zhang and M. Glasbeek	254 (2000) 319
Nonlinear responses (incl. optical)	
Channels of the exciton-exciton annihilation in one-dimensional aggregates at low temperature, V.A. Malyshev, G.G. Kozlov, H. Glaeske and KH. Feller	254 (2000) 31
A novel approach to calculation of the second-order nonlinear optical susceptibilities of organic crystals based on energy-band theory, XL. Zhu, XZ. You and	
Y. Zhang	254 (2000) 287
Reactions (incl. dissociation)	
Temperature dependence of fast neutral-neutral reactions: a triatomic model study, A. Faure, L. Wiesenfeld and P. Valiron	254 (2000) 49
A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the	234 (2000) 49
CO ₂ +H ₂ →HCOOH gas phase process, H. Chevreau, E. Boullant, C. Dézarnaud- Dandine and A. Sevin	254 (2000) 99
Reactions of ground state Ti atoms with NO: insertion versus complexation. An IR matrix isolation study, L. Krim, C. Prot, E.M. Alikhani and L. Manceron	254 (2000) 267
-isolated molecules	
The unimolecular dissociation of 2-butenenitrile: measurements of the CN elimination channel using FM Doppler spectroscopy, R. Li, A. Derecskei-Kovacs and S.W. North	254 (2000) 309
-condensed phase Role of inertial and non-Markovian effects on activated barrier crossing dynamics for	
charge transfer reactions in solution, A. Samanta and S.K. Ghosh Kinetic energy distributions for O and metastable CO produced by electron	254 (2000) 39
stimulated desorption from condensed CO ₂ , M. Tronc, R. Azria, Y. Le Coat, P. Cloutier and L. Sanche	254 (2000) 69
Electron transfer	
Anisotropic double exchange in orbitally degenerate mixed valence systems, J.J. Borras- Almenar, J.M. Clemente-Juan, E. Coronado, A.V. Palii and B.S. Tsukerblat	254 (2000) 275
Proton and hydrogen atom transfer	
Semiempirical modeling free energy surfaces for proton transfer in polar aprotic solvents, M.V. Vener, I.V. Rostov, A.V. Soudackov and M.V. Basilevsky	254 (2000) 249

Surface chemical physics

-desorption

Kinetic energy distributions for O⁻ and metastable CO^{*} produced by electron stimulated desorption from condensed CO₂, M. Tronc, R. Azria, Y. Le Coat, P. Cloutier and L. Sanche

254 (2000) 69

Structure of solids, liquids and glasses

Structural properties and quantum effects in protonated helium clusters. II. Quantum Monte Carlo calculations for the smaller aggregates, B. Balta, F.A. Gianturco and F. Paesani

254 (2000) 215